

Warning! If you are
a physicist, you write
everything differently.

Polar/Cylindrical: r becomes ρ ,
 θ becomes φ .

Spherical: ρ becomes r , θ becomes
 φ , φ becomes θ

I assume there are good reasons
for this

Example 1. (physical chemistry)

$$\text{Let } f(\rho, \theta, \varphi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-\rho/a_0}$$

be the atomic orbital of
a 1s hydrogen atom.

Here, "1" = energy level

"s" = shape of orbit (sphere)

" a_0 " = Bohr radius

$$\approx 5.2917 \times 10^{-11} \text{ m}$$

The integral of the square of f over all of 3-space represents the probability of finding the hydrogen atom at **all** possible radii values ρ . Therefore,

we should find

$$\int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} (f(\rho, \theta, \varphi))^2 \rho^2 \sin\varphi d\varphi d\theta d\rho = 1$$

Check:

$$\int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} \left(\frac{e^{-p/a_0}}{\sqrt{\pi a_0^3}} \right)^2 p^2 \sin\varphi \, d\varphi \, d\theta \, dp$$

$$= 2\pi \int_0^{\infty} \frac{e^{-2p/a_0} p^2}{\pi a_0^3} dp \cdot \int_0^{\pi} \sin\varphi \, d\varphi$$

$$= \frac{2}{a_0^3} \int_0^{\infty} e^{-2p/a_0} p^2 dp \left(-\cos\varphi \Big|_0^{\pi} \right)$$
$$= \frac{4}{a_0^3} \int_0^{\infty} e^{-2p/a_0} p^2 dp$$

Then

$$\frac{4}{a_0^3} \int_0^{\infty} e^{-2p/a_0} p^2 dp$$

$$= \frac{4}{a_0^3} \lim_{t \rightarrow \infty} \int_0^t e^{-2p/a_0} p^2 dp$$

integrate by parts
- tabular

u	dv
p^2	e^{-2p/a_0}
$2p$	$e^{-2p/a_0} (-a_0/2)$
2	$e^{-2p/a_0} (a_0/2)^2$
0	$e^{-2p/a_0} (-a_0/2)^3$
	e

We get

$$\frac{4}{a_0^3} \lim_{t \rightarrow \infty} \left(-\frac{a_0}{2} e^{-2t/a_0} \right) \left(t^2 - \frac{2ta_0}{2} + \frac{a_0^2}{2} \right) \Big|_0^t$$

$$= \frac{4}{a_0^3} \left(\lim_{t \rightarrow \infty} \left(-\frac{a_0}{2} e^{-2t/a_0} \right) \left(t^2 - \frac{2ta_0}{2} + \frac{a_0^2}{2} \right) - \left(-\frac{a_0^3}{4} \right) \right)$$

The limit is zero (l'Hopital's rule),

so we get

$$\frac{4}{a_0^3} \cdot \frac{a_0^3}{4} = \boxed{1}$$

Notes 1) If the orbital is only dependent on ρ , you always end up with

$$4\pi \int_0^{\infty} \rho^2 f(\rho)^2 d\rho$$

2) Hydrogen is easiest (1 electron)

If you can ionize down to one electron, then the integrals that occur look much like hydrogen